Characterization of Carbon Nanotubes under Deformation

Richard L. Jaffe, Liu Yang, Jie Han, M. P. Anantram

Ongoing nanotechnology research at Ames Research Center is aimed at developing revolutionary small-scale electronic devices and sensors to meet the requirements of future NASA missions. Carbon Nanotubes (CNT) are hollow cylinders of graphitic carbon atoms; the cylinders have diameters of ~0.001 microns and lengths of up to several microns (more than 100 times smaller than the components of today's microprocessors). Depending on the orientation of the hexagonal carbon rings in the tube surface, some CNTs have metallic properties (that is, the band gap is zero) and others are semiconductors (that is, the band gap is finite, but less than 1 electron volt).

Because of their varying electronic properties and very small size, CNT components are expected to have an important role in the development of future electronic devices. In addition, CNTs have extraordinarily large tensile modulus and tensile strength, which places them among the strongest materials known. These attributes make them promising candidates for reinforcing fibers and for microelectronic-mechanical sensors (MEMS). Single-CNT transistors (shown schematically in figure 1) have been fabricated and tested under ideal laboratory conditions, but it is not known whether they will function under typical operating conditions of integrated circuits. Previously, modeling studies were carried out to characterize idealized CNT electronic devices. This year, research focused on characterizing electronic devices and sensors under realistic operating conditions where the CNTs are bent, flattened, and twisted by their interactions with substrates, metal contacts, and other devices.

Electronic properties of stretched, compressed, and bent CNTs have been studied, using a full-valence electron tight-binding model to calculate the electronic density of states (DOS), bandgap and conductance. Selected results for stretched and compressed nanotubes are illustrated in figure 2.

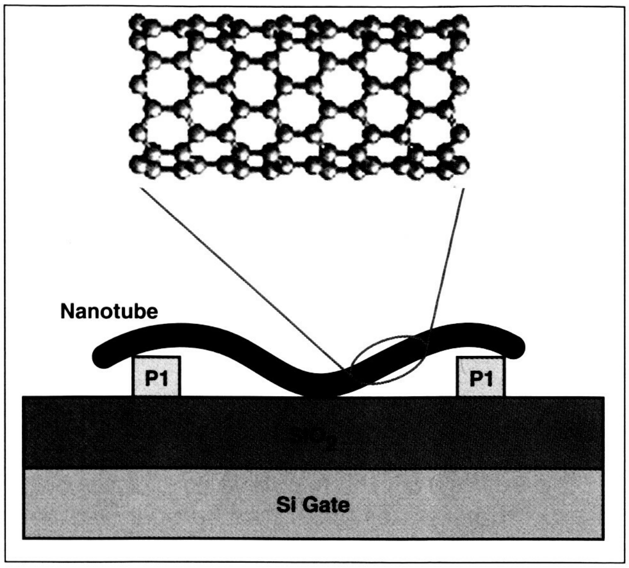

Fig. 1. Schematic diagram of a single carbon nanotube transistor. The source and drain potentials are applied at the platinum contacts, and the gate voltage from the underlying silicon controls the operation of the device.

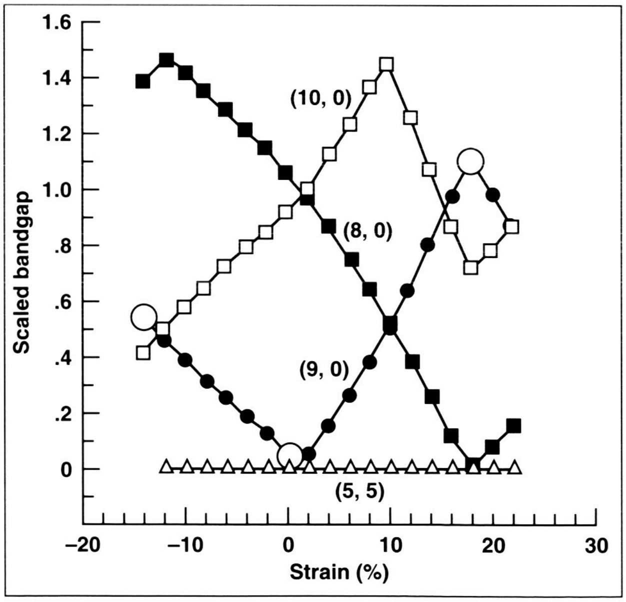

Fig. 2. Variation of computed band gap as a function of tensile strain for several different carbon nanotubes; negative strain represents compression, and positive strain represents tension.

Similar results have been found for other deformations. We find that some metallic-like nanotubes (labeled 5,5) remain conducting even when subjected to large compressive or tensile strain, as evidenced by their bandgaps remaining zero. However, other conducting tubes (labeled 9,0) develop sizeable band gaps under these conditions. Finally the band gaps of semiconducting tubes (8,0 and 10,0) are found to be very sensitive to the applied strain. Metallic nanotubes, such as the (5,5), retain their electronic properties even when subjected to large deformations; as a result, they are promising candidates for use in CNT-based electronic devices. On the other hand, other conducting tubes, such as the (9,0), are good candidates for MEMS devices, because their conductivity decreases markedly with increasing tensile strain. Optimal performance of CNT devices and sensors will be achieved by selecting the correct type of nanotube for the particular application.

Point of Contact: R. Jaffe
(650) 604-6458
rjaffe@mail.arc.nasa.gov

Computational Quantum Optoelectronics for Information Technology

C. Z. Ning, S. C. Cheung, P. M. Goorjian, J. Li, A. Liu

The interaction between laser light and semiconductor nanostructures is the basis for current and future optoelectronics-based information technology. The objective of the Computational Quantum Optoelectronics (CQP) project at Ames Research Center is to explore new optoelectronic devices, to study speed and size limits imposed by fundamental physics principles, and to design and optimize the performance of existing devices to meet NASA's needs in information technology. During FY99 the project made significant accomplishments in three areas: comprehensive semiconductor laser simulation, ultrafast laser modulation with a terahertz heating field, and terahertz wave generation in semiconductor quantum wells.

In terms of comprehensive laser simulation, the focus in FY99 was on the so-called vertical-cavity surface-emitting laser (VCSEL). Ames researchers have developed a comprehensive simulation code using finite-difference methods in time and two-dimensional space domain. The model takes into account the quantum-well structure information and the material composition of a given VCSEL structure design. The effects of the detailed Coulomb interactions of charged carriers are also included. Since researchers directly solve the resulting partial differential equations numerically, VCSELs of different designs are treated with the same ease, such as those with gain confinement or index confinement, or devices of different current contact shapes. Also, time-evolution of VCSEL spatial modes on a picosecond scale are resolved. This type of space-time-resolved simulation is especially important when VCSELs are subject to injection current modulation, as is the case in VCSEL-based interconnects. Figure 1 shows the output laser intensity patterns at four different pumping levels for a VCSEL with an annular current contact.

In the area of ultrafast laser modulation, researchers have investigated the possibility of increasing the communication bandwidth by utilizing the much faster process of heating the electron-hole gas in a semiconductor with an electrical field. Detailed investigation has shown the feasibility and limitations of using such an approach. Researchers have investigated the underlying physical processes of electron-hole plasma interacting with semiconductor lattice vibrations when heated by an applied electrical field with frequency up to a few terahertz. They developed a detailed model to study laser modulation under such a terahertz-heating field. The results show that this method allows a modulation of semiconductor lasers at frequencies from tens of gigahertz (10^9 Hz) to 1 terahertz (10^{12} Hz). Even though it is a theoretical result at this stage, the approach indicates some fundamental advantages of this new modulation strategy over existing approaches.

Another closely related area of research in the overall effort in quantum optoelectronics is terahertz generation. We have investigated two possibilities using carefully designed quantum-well structures for